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Status of Evaluated Data Files for ^{238}U in the Resonance Region

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Abstract
Experimental data and evaluated data libraries related to neutron induced reaction cross sections for ^{238}U in the resonance region are reviewed. Based on this review a set of test files is produced to study systematic effects such as the impact of the upper boundary of the resolved resonance region (RRR) and the representation of the infinite diluted capture and in-elastic cross section in the unresolved resonance region (URR). A set of benchmark experiments was selected and used to verify the test files. Based on these studies recommendations for a new evaluation have been defined.

STATUS OF EVALUATED DATA FILES FOR ^{238}U
IN THE RESONANCE REGION

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Executive summary

Experimental data and evaluated data libraries related to neutron induced reaction cross sections for ^{238}U in the resonance region are reviewed. Based on this review a set of test files is produced to study systematic effects such as the impact of the upper boundary of the resolved resonance region (RRR) and the representation of the infinite diluted capture and in-elastic cross section in the unresolved resonance region (URR). A set of benchmark experiments was selected and used to verify the test files. Based on these studies recommendations to perform a new evaluation have been defined.

This report has been prepared in support to the CIELO (Collaborative International Evaluated Library Organisation) project. The objective of this project is the creation of a world-wide recognised nuclear data file with a focus on six nuclides, i.e. ^{1}H, ^{16}O, ^{56}Fe, ^{235}U, ^{238}U and ^{239}Pu. Within the CIELO project, the Joint Research Centre (JRC) at Geel (B) is in charge of the production of an evaluated cross section data file for neutron induced reactions of ^{238}U in the resonance region.

Contents

1. Introduction

In most operating nuclear power reactors more than 90% of the fuel in a nuclear power reactor consists of ^{238}U. Therefore, cross sections for neutron induced reactions with ^{238}U as target nucleus are of primary importance when accurate neutron transport calculations are required. Due to the role of these cross sections for nuclear energy and criticality safety applications, ^{238}U is chosen as one of the key nuclides within the CIELO (Collaborative International Evaluated Library Organisation) project [1]. The objective of this project is the creation of a world-wide recognised nuclear data file with a focus on six nuclides, i.e. ^{1}H, ^{16}O, ^{56}Fe, ^{235}U, ^{238}U and ^{239}Pu. Different research groups in various parts of the world are working on improved evaluated data and their uncertainties for these nuclides.

Within the CIELO project, the Joint Research Centre (JRC) at Geel (B) is in charge of the production of an evaluated cross section data file for neutron induced reaction of ^{238}U in the resonance region. The production of such a file includes different steps:

- review of experimental data and evaluated data libraries;
- recommendation for additional experiments;
- production of an evaluated data file, including full covariance data; and
- validation based on results of benchmark experiments.

In this report experimental data and evaluated data libraries related to neutron induced reaction cross sections for ^{238}U in the resonance region are reviewed. Based on this review a set of test files was produced to study systematic effects, such as the impact of the upper boundary of the resolved resonance region (RRR) and the representation of the infinite diluted capture and in-elastic cross section in the unresolved resonance region (URR). A set of benchmark experiments was selected and used to verify the test files.

This report has been prepared by the JRC. However, it results from an extensive collaboration of specialists in cross section measurements, neutron resonance spectroscopy, nuclear reaction theory and integral benchmark experiments. It involves scientists from international organisations and national institutes:

- European Commission, Joint Research Centre, Geel (Belgium)
- International Atomic Energy Agency, Vienna (Austria)
- OECD Nuclear Energy Agency, Issy-les-Moulineaux (France)
- Commissariat à l'Energie Atomique, Cadarache (France)
- Institut de Radioprotection et de Sûreté Nucléaire, Fontenay-aux-Roses (France)
- Institute for Nuclear Research and Nuclear Energy, Sofia (Bulgaria)
- Institute of Physics and Power Engineering, Obninsk (Russia)
- Korea Atomic Energy Research Institute, Daejeon (Korea).

2. Evaluated data files for ^{238}U in the resonance region

In this section experimental cross section data reported in the literature and their relation to evaluated data files for neutron induced reactions of ^{238}U in the resonance region are discussed. The section is subdivided in a study of cross sections in the RRR and URR. Based on these studies a set of test files was produced.

2.1 Evaluated data files in the RRR

The first evaluation for ^{238}U in the RRR based on a full resonance shape analysis was carried out by Moxon et al. [2] using the REFIT code [3]. They derived parameters for individual resonances up to 10 keV from a simultaneous least squares fit to transmission [4-8], capture [9,10] and fission [11] cross section data obtained from measurements at ORELA. The transmission data of Olsen et al. [4,5] resulted from experiments at a 40 m and 150 m station using 7 different samples with areal densities ranging from 0.0002 at/b to 0.175 at/b. The capture data of de Saussure et al. [9] and Macklin et al. [10] were obtained from measurements with the ORELAST detector at 40 m and 150 m, respectively. The fission widths were derived from the fission areas measured by Difilippo et al. [11]. Moxon et al. [2] noted that the capture data of de Saussure et al. [9] and Macklin et al. [10] were inconsistent with the transmission results. The data of de Saussure et al. [9] above the 6.67 eV resonance were renormalized by a factor of ~ 0.9. The capture data of Macklin et al. [10] required a normalization factor of ~ 1.10. They both required a background correction that was larger than a 50 mb equivalent cross section. The parameters of strong s-wave resonances below 300 eV for which both the neutron width Γ_n and radiation width Γ_γ were determined are specified in Table 1, together with the capture kernel K_γ:

$$K_\gamma = \frac{\Gamma_n \Gamma_\gamma}{\Gamma_n + \Gamma_\gamma}. \tag{1}$$

The average radiation width for resonance below 300 eV is ~ 23.5 meV. The evaluation of Moxon et al. [2] was adopted in JEF-2.2 and taken over in JENDL 3.3 and ENDF/B-VI.1.

Table 1. Parameters of strong s-wave resonances resulting from an evaluation reported in Moxon et al. [2] and Derrien et al. [12]. The capture kernels K_γ (Eq. 1) are also given.

	Moxon et al. [2]					Derrien et al. [12]		
E_r (eV)	Γ_n (meV)		Γ_γ (meV)		K_γ (meV)	Γ_n (meV)	Γ_γ (meV)	K_γ (meV)
6.67	1.493	(0.002)	23.00	(0.04)	1.402	1.476	23.00	1.387
20.87	10.258	(0.009)	22.91	(0.04)	7.085	10.09	22.86	7.000
36.68	34.129	(0.023)	22.89	(0.05)	13.701	33.55	23.00	13.645
66.03	24.605	(0.041)	23.36	(0.12)	11.983	24.18	23.31	11.869
80.75	1.865	(0.022)	23.42	(0.58)	1.727	1.874	23.39	1.735
102.56	77.704	(0.195)	23.42	(0.20)	17.996	70.77	24.08	17.967
116.90	25.486	(0.093)	23.00	(0.26)	12.090	25.35	22.28	11.858
165.32	3.367	(0.008)	25.76	(2.94)	2.978	3.19	24.37	2.821
189.68	173.200	(0.320)	22.38	(0.40)	19.819	170.18	23.58	20.710
208.52	51.110	(0.200)	23.94	(0.31)	16.303	49.88	22.84	15.666
237.40	27.159	(0.160)	25.80	(0.84)	13.231	26.45	25.18	12.900
273.67	25.78	(0.180)	25.17	(1.18)	12.736	24.87	24.41	12.319
291.01	16.873	(0.170)	21.00	(2.08)	9.356	16.54	23.23	9.661

The parameters of Moxon et al. [2] are the basis of the evaluation reported by Derrien et al [12] in 2005. Derrien et al. [12] extended the upper limit of the RRR by including the transmission data of Harvey et al. [13] and adding resonances based on a level statistical analysis. The data of Harvey et al. [13] resulted from experiments at a 200 m station of ORELA with 3 samples (0.0124 at/b, 0.0400 at/b and 0.175 at/b). Derrien et al. [12] also included in their analysis the energy dependence of the capture cross section in the thermal energy region derived by Corvi and Fioni [14] and transmission measurements at 24 K and 294 K from Meister et al. [15]. The experiments of Corvi and Fioni [14] and Meister et al. [15] were carried out at GELINA. The spin assignments of Gunsing et al. [16] were taken into account. Derrien et al. [12] confirmed that the capture data of de Saussure et al. [9] and Macklin et al. [10] suffered from a systematic bias effect and applied normalization correction factors which were very similar to those of Moxon et al. [2]. These corrections are not compatible with the uncertainties quoted by the authors, i.e. about 5 - 10 % by de Saussure et al. [9] and 8 % by Macklin et al. [10]. The parameters obtained by Derrien et al. [12] for strong s-wave resonances below 300 eV are listed in Table 1. The neutron widths and capture kernels of Moxon et al. [2] are ~ 1% and ~ 2.5 %, respectively, larger compared to those of Derrien et al. [12] for the resonances in Table 1. The average radiation width for resonances below 300 eV is ~ 23.5 meV.

The resonance parameters (i.e. energy, neutron and radiation width) of Derrien et al. [12] have been adopted in ENDFB/VII.1 and JENDL-4.0. The file was taken over in JEFF-3.2 after some modifications. For the production of JEFF-3.2 a level statistical analysis based on the Wigner and Porter-Thomas distributions was performed by Litaize et al. [17]. This analysis included Dyson F-statistic and Mehta-Dyson Δ_3 tests. The original parity assignments of the 551 eV and 2919 eV resonances were changed into ℓ= 1 and 0, respectively, based on the results of this analysis.

Unfortunately the fission widths in ENDFB/VII.1, JENDL 4.0 and JEFF-3.2 were adopted from JEF-2.2 without considering differences in neutron and capture widths. Consequently some of the fission areas are not consistent with those of Difilippo et al. [11]. The fission areas reported by Difilippo et al. [11] are limited to resonance energies $\leq$ 1200 eV. It is not clear from which data the parameters for higher energy resonances in the different libraries were derived.

An overview of evaluated data libraries for ^{238}U and their relation to the work of Moxon et al. [2] and Derrien et al. [12] is given in Table 2. The BROND-2.2 file can be considered as an independent evaluation. Unfortunately, the original evaluation report is in Russian and has not been translated. Table 2 includes the scattering, capture and fission cross sections at the thermal energy together with coherent scattering lengths derived from the elastic scattering cross section at thermal energy. These values can be compared with the coherent scattering lengths in Table 3, which were obtained from dedicated experiments [18 - 21]. Most of the evaluations are consistent with the value (8.63 $\pm$ 0.04) fm of Koester et al. [19]. The thermal capture cross section (2.683 $\pm$ 0.012) b recommended by Trkov et al. [22] was used in ENDF/B-VII.1 to adjust the contribution of the external levels. This value is ~ 1.3% lower compared to the one adopted in the evaluation of Moxon et al. [2].

Table 2. Relation between the main evaluated data libraries and the evaluation reports of Moxon et al. [2], Derrien et al. [12] and Fröhner [23,24]. The recommended scattering σ(n,n), capture σ(n,γ) and fission σ(n,f) cross sections at thermal energy and coherent scattering length (b_c) derived from σ(n,n) are given.

Library	Reference		Cross sections at 2200 m/s			b_c
	RRR	URR	σ(n,n)	σ(n,γ)	σ(n,f)	
BROND -2.2			8.916 b	2.714 b	0 b	8.459 fm
ENDF/B-VI.8	JEF-2.2	JEF-2.2	9.376 b	2.718 b	12 μb	8.674 fm
ENDF/B-VII.1	Derrien et al. [12]	Fröhner [23,24]	9.299 b	2.683 b	12 μb	8.638 fm
JEF-2.2	Moxon et al. [2]	Fröhner [23,24]	9.376 b	2.718 b	12 μb	8.674 fm
JEFF-3.2	Derrien et al. [12]	Fröhner [23,24]	9.437 b	2.684 b	12 μb	8.702 fm
JENDL-3.3	JEF-2.2	[25-32]	9.380 b	2.718 b	12 μb	8.676 fm
JENDL-4.0	ENDF/B-VII.1	JENDL-3.3	9.299 b	2.683 b	12 μb	8.638 fm

Table 3. Coherent scattering lengths reported in the literature.

Reference	Scattering length	Method
Roof et al. [18]	(8.50 $\pm$ 0.50) fm	Bragg diffraction
Willis et al. taken from [19]	(8.50 $\pm$ 0.06) fm	Bragg diffraction
Atoji [20]	(8.55 $\pm$ 0.06) fm	Bragg diffraction
Koester et al. taken from [19]	(8.63 $\pm$ 0.04) fm	Cristiansen filter
Boeuf et al. [21]	(8.407 $\pm$ 0.007) fm	Interferometer

The scattering and capture cross sections of the independent libraries, i.e. BROND 2.2, JEF-2.2, and ENDF/B-VII.1, are compared in Figure 1 and Figure 2. To facilitate the comparison the cross sections of BROND-2.2 and JEF-2.2 are plotted relative to those of ENDF/B-VII.1. In addition, a 172 energy group structure optimised for Light Water Reactor transport calculations was applied.

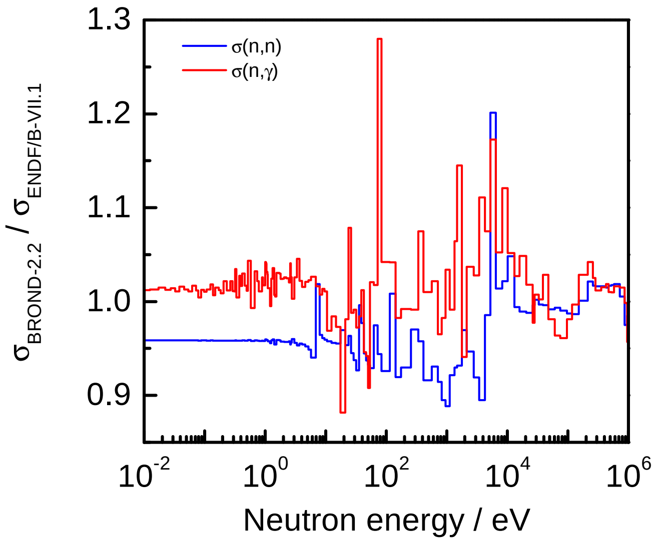

Figure 1 Ratio of the elastic scattering and capture cross section in BROND-2.2 and those in ENDF/B-VII.1 as a function of neutron energy. The cross sections have been calculated in a 172 group energy structure.

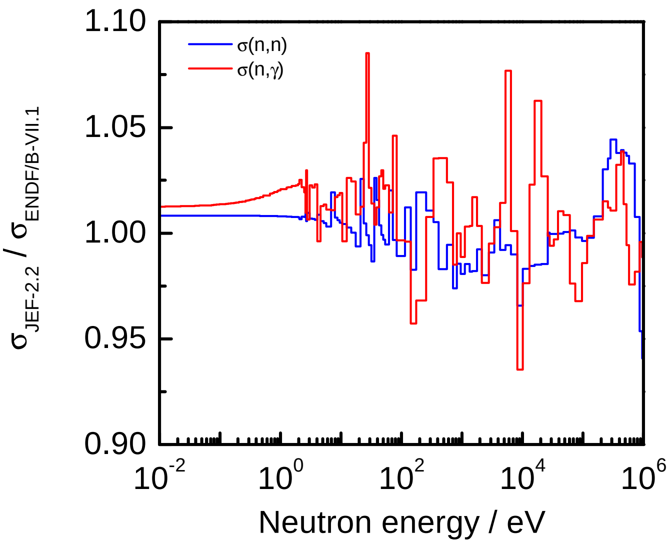

Figure 2 Ratio of the elastic scattering and capture cross section in JEF-2.2 and those in ENDF/B-VII.1 as a function of neutron energy. The cross sections have been calculated in a 172 group energy structure.

2.2 Evaluated data files in the URR

Most of the evaluated data libraries refer to the cross sections in the URR evaluated by Fröhner [23,24]. This evaluation is based on an analysis of experimental data using the Hauser-Feshbach theory with width fluctuations (HF+WF). A similar evaluation was carried out by Maslov et al. [25] and Courcelle et al. [26]. The total cross section resulting from these evaluations are mainly determined by the data of Uttley et al. [27], Whalen et al. [28], Konovov and Poletaev [29], Poenitz et al. [30] and Tsubone et al. [31]. The total cross sections of Harvey et al. [13] have only been taken into account in the analysis of Courcelle et al. [26]. The capture cross section is predominantly determined by the cross section of Moxon [32, 33] and Kazakov et al. [34]. It should be noted that the data of Moxon in the EXFOR entry 22541 [33] result from a revision by Moxon of the original data [33]. The capture cross sections of de Saussure et al. [9] and Macklin et al. [10] deviate by about 10% from the one recommended by Fröhner [23,24]. Therefore, these cross sections were not included in the evaluation of Fröhner [23,24] and Courcelle et al. [26].

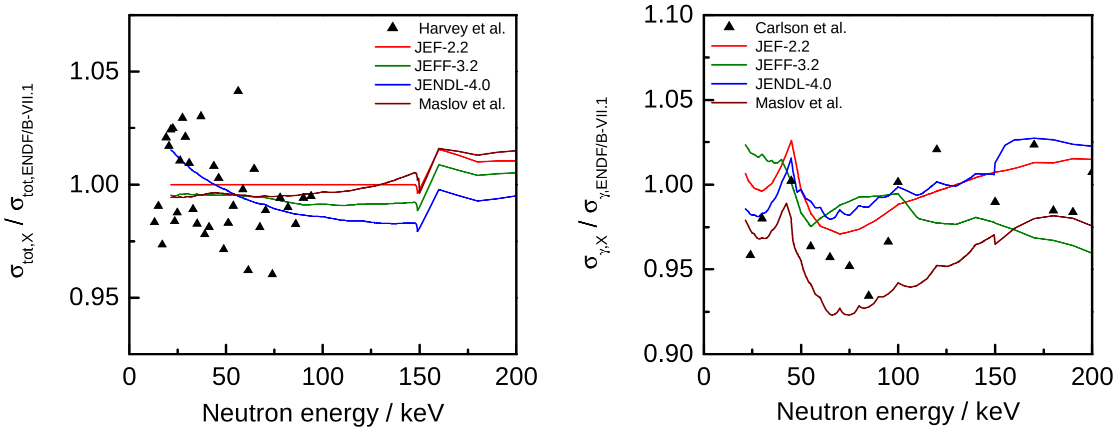

Figure 3 Ratio of the total (left) and capture (right) cross sections in evaluated data libraries (JEF-2.2, JEFF-3.2, JENDL-4) and those in ENDF/B-VII.1 as a function of neutron energy. The ratio of the cross sections recommended by Maslov et al. [25] and ENDF/B-VII.1 are also given. For the total cross section the ratio of the experimental data of Harvey et al. [13] is given while for the capture reaction the one recommended by Carlson et al.[35], which is based on a least squares adjustment of experimental data.

A comparison of the evaluated total and capture cross sections in the URR is given in Figure 3. The total and capture cross sections relative to those in ENDF/B-VII.1 are plotted as a function of neutron energy. Although most of the libraries are based on the work of Fröhner [23,24] differences between the recommended cross sections are observed. Figure 3 illustrates that the evaluated total cross sections are systematically higher compared to the cross section derived from transmission measurements of Harvey et al. [13]. These data were included in the evaluation of Derrien et al. [12] for the RRR. However, they were not considered in any of the evaluations for the main evaluated data libraries. The comparison of capture cross sections in Figure 3 includes the one of Carlson et al. [35]. The latter was produced as part of the standards project and results from a least-squares adjustment of experimental data using the GMA code developed by Poenitz [36]. This figure reveals difference of up to 5% between the capture cross sections in the evaluated data libraries and the one recommended by Carlson et al. [35]. The ENDF/B-VII.1 capture cross section is on average ~ 2.0 % higher compared to the one of Carlson et al. [35] in the energy region between 20 keV and 150 keV.

2.3 Test files for ^{238}U in the resonance region

A set of test files was produced to verify systematic effects in the resonance region. They were based on the resolved resonance parameters in JEFF-3.2, the average capture cross section recommended by Carlson et al. [35] results of optical model calculations using the Dispersive Coupled Channel Optical Model Potential (DCCOM) of Quesada et al. [37], and inelastic neutron scattering data of Capote et al [38] that consider compound-direct interference effects. The transmission coefficients and shape elastic cross section from the optical model were used to derive average parameters, i.e. neutron strength functions and hard sphere scattering radius, in terms of a full ENDF compatible URR model following the procedure that was applied for ^{232}Th [39] and ^{197}Au [40,41]. The capture transmission coefficients were obtained from a fit to the capture cross section of Carlson et al. [35].

Eight different files were produced. They differ in the infinitely diluted capture and inelastic scattering cross sections and the upper boundary of the resolved resonance region, i.e. 10 keV and 20 keV. The infinitely diluted capture cross section was adopted from the GMA analysis reported by Carlson et al. [35] or calculated based on average resonance parameters resulting from a fit to the data of Carlson et al. [35]. The inelastic cross section was obtained by adding its compound component calculated from the average parameters and a direct component based on the DCCOM or by adopting the one recommended in a recent evaluation of Capote et al. [38]. An overview of the different test files is given in Table 4. For each version the corresponding ACE files were produced.

Table 4. Description of the different test files produced for the cross sections in the URR.

File	σ(n,γ)	σ(n,n'γ)	Upper energy boundary RRR
G10-1	Calculated	Calculated	10 keV
G20-1	Calculated	Calculated	20 keV
G10-2	Adopted from [35]	Calculated	10 keV
G20-2	Adopted from [35]	Calculated	20 keV
G10-3	Calculated	Adopted from [37,38]	10 keV
G20-3	Calculated	Adopted from [37,38]	20 keV
G10-4	Adopted from [35]	Adopted from [37,38]	10 keV
G20-4	Adopted from [35]	Adopted from [37,38]	20 keV

3. Validation

3.1. Validation by energy dependent cross section data

A first validation exercise was based on an analysis of the thick sample transmission data of Olsen et al. [4] and Harvey et al. [13]. As mentioned in Ref. [42], thick sample transmission data are among the most accurate data to validate resonance parameters.

The performance of the parameters for the RRR was verified by comparing the experimental transmission data of Olsen et al. [4] with the theoretical transmission calculated from the resonance parameters recommended by Derrien et al. [12]. In the calculations the resonance shape analysis code REFIT [3] was used.

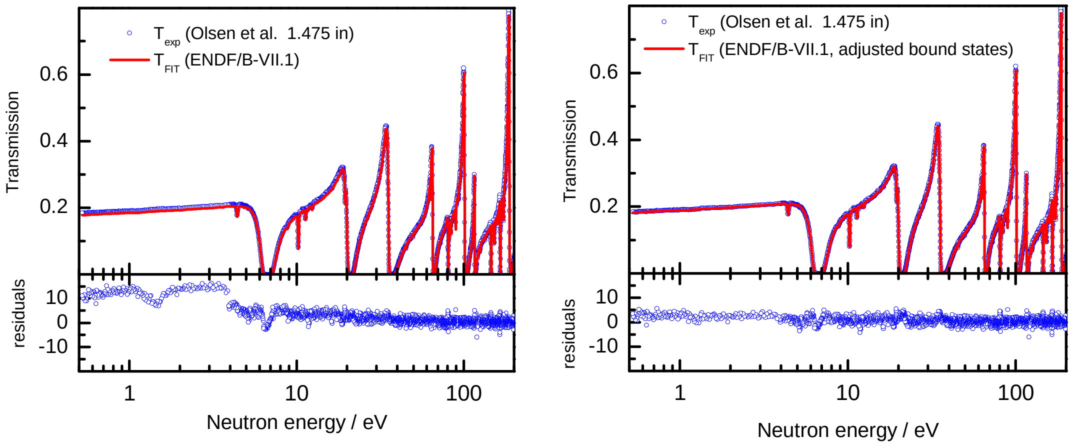

Figure 4. Comparison of the experimental (T_{exp}) and theoretical (T_{FIT}) transmission as a function of neutron energy. The experimental data result from transmission measurements at ORELA obtained with a thick ^{238}U sample (areal density = 0.175 at/b). The theoretical transmission results from calculations with REFIT using the ENDF/B-VII.1 resonance parameters (left) and a file based on ENDF/B-VII.1 with the parameters of the two bound states (i.e. those of – 7 eV and – 33 eV in ENDF/B-VII.1) adjusted (right).

The results in Figure 4, which compares the experimental and theoretical transmission for the uranium sample with a 0.175 at/b areal density, illustrates that when using the parameters of Derrien et al. [12] the theoretical and experimental transmission are not consistent. This suggests that Derrien et al. [12] have applied a normalization correction on the experimental transmission data. Figure 5 (right) shows that good agreement between experimental and theoretical transmission can also be obtained by adjusting the parameters of the bound states without renormalizing the experimental data. The theoretical transmission after an adjustment of the resonance energy and neutron widths of two bound states, i.e. of the – 7 eV and – 33 eV levels in Ref. [12], is in good agreement with the experimental transmission and no additional re-normalization of the data is required. To confirm the parameters of the bound states additional transmission measurements are recommended and a comparison with experimental benchmarks sensitive to the thermal energy region is required.

To study the impact of the upper boundary of the RRR the experimental transmission data of Harvey et al. [13] obtained with the 0.175 at/b sample were compared with results of Monte Carlo simulations based on the G10-3 and G20-3 files with an upper boundary for the RRR of 10 keV and 20 keV, respectively. Both the experimental and theoretical transmissions were derived in the SAND-II 640 group structure that is frequently used for dosimetry applications. The results in Figure 5 show the good agreement between the experimental and theoretical transmission for both files. They also indicate that whenever such a group structure is required an upper boundary of 20 keV for the RRR can be recommended.

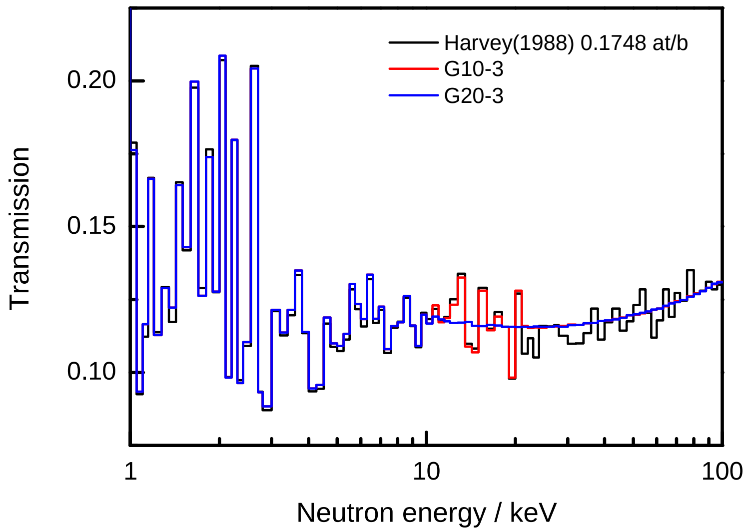

Figure 5. Comparison of the experimental and theoretical transmission as a function of neutron energy. The experimental data result from transmission measurements of Harvey et al. [13] at a 200 m transmission station of ORELA using a ^{238}U sample with an areal density of 0.175 at/b. The theoretical transmission results from Monte Carlo simulations based on the G10-3 and G20-3 files.

3.2 Validation by integral benchmark experiments

3.2.1 Validation activities of Subgroup 22

The performance of the resonance parameter files produced by Moxon et al. [2] and Derrien et al. [12] was investigated by Subgroup 22 of WPEC [43]. They demonstrated the value of the LEU-MET-THERM-006 experiments to validate the capture cross section in resonance region. These experiments are included in the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP) [44]. Using the parameters of Derrien et al. [12] the reactivity increased by about 600 x 10^{-5} (or 600 pcm) due to a decrease in calculated ^{238}U reaction rate. In addition, the calculated k_{eff} as function of $^{238}U(n,\gamma)$ fraction was consistent with the experimental data. An overestimation of the $^{238}U(n,\gamma)$ cross section can explain the difference between calculated and experimental spectral indices for several thermal lattice experiments which were carried out at the EOLE facility [45] and the overestimation of the $^{239}Pu/^{238}U$ ratio using the JEF-2.2 evaluation (see Ref. [43] for more details and relevant references).

3.2.2 Validation of test files by IAEA

The on-line version of ICSBEP/DICE was applied to identify benchmark experiments which are sensitive to the capture cross section of ^{238}U in the thermal energy region and in the URR.

The experiments sensitive to cross sections in the thermal energy region are listed in Appendix A. As expected from the work of Subgroup 22, they include the LEU-MET-THERM-006 set. These benchmarks can be used to verify the impact of the change in the parameters of the bound states. Unfortunately the MCNP input models are not available and the impact of changes in resonance parameters of the bound states could not be verified.

Integral experiments from the ICSBEP Handbook [44] with a high sensitivity to the cross sections for ^{238}U in the energy range between 10 keV and 20 keV are listed in Appendix B. For six of them MCNP input files are available. For these benchmarks, which are listed in Table 5, the reactivity k_{eff} was calculated based on four cross section files [46]:

- ENDF/B-VII.1 — ENDF/B-VII.1 library supplied with the MCNP-6.1 package
- U238_ib36 — the IAEA starter file for ^{238}U version ib36 [46]
- U238_ib36_G10-3 — the IAEA starter file for ^{238}U with the file G10-3 for the URR
- U238_ib36_G20-3 — the IAEA starter file for ^{238}U with the file G20-3 for the URR

The capture cross section in ENDF/B-VII.1 and U238_ib36 are the same, the one in U238_ib36_G10-3 and U238_ib36_G20-3 result from the evaluation of Carlson et al. [35].

Table 5. Integral benchmark experiments with a high sensitivity to the ^{238}U cross sections between 10 keV and 20 keV. Only experiments from the ICSBEP Handbook [44] for which MCNP input files are available are listed. The first column is used as identification number in Figure 6.

Number	ICSBEP Id	Short name	Common name	$k_{eff,E}$	$u_{keff,E}$
1	MIX-MET-INTER-004	mmi004	ZPR-3/53	0.9757	0.0023
2	IEU-COMP-INTER-001	ici001	ZPR-6/6A	0.9939	0.0023
3	MIX-COMP-FAST-001	mcf001	ZPR-6/7	0.9866	0.0023
4	MIX-COMP-FAST-001	mcf005	ZPR-9/31	0.9913	0.0023
5	MIX-COMP-FAST-001	mcf006	ZPPR-2	0.9889	0.0021
6	MIX-MISC-FAST-001.9	mmf001-09	BSF-31-4	1.0188	0.0072

The results of this exercise are presented in Figure 6 and Table 6. Figure 6 plots the difference between the calculated $k_{eff,C}$ and experimental reactivity $k_{eff.,E}$ as a function of the experiment number together with the residual which is defined by:

$$R = \frac{k_{eff,C} - k_{eff,E}}{u_{keff,E}}, \tag{2}$$

where $u_{keff,E}$ is the uncertainty on the experimental value. From the data in Figure 6 the average difference between calculated and experimental reactivity and χ^2-value, which is defined by:

$$\chi^2 = \sum \left(\frac{k_{eff,C} - k_{eff,E}}{u_{keff,E}} \right)^2, \tag{3}$$

were calculated. For the above mentioned test files, these values are listed in Table 6.

The data in Figure 6 and Table 6 show that there is almost no difference between the results obtained with the U238_ib36_G10-3 and U238_ib36_G20-3 file. Hence, even for the benchmarks in Table 5, which have a high sensitivity for the cross sections in the region between 10 keV and 20 keV, the increase in upper boundary of the RRR from 10 keV to 20 keV has almost no impact. The k_{eff} obtained with calculations based on the G10-3 and G20-3 files is larger compared to the one derived from the calculations with the ENDF/B-VII.1 and U238_ib36 file. This increase in reactivity can be due to a lower capture cross for the file based on the cross section of Carlson et al. [35], as shown in Figure 3.

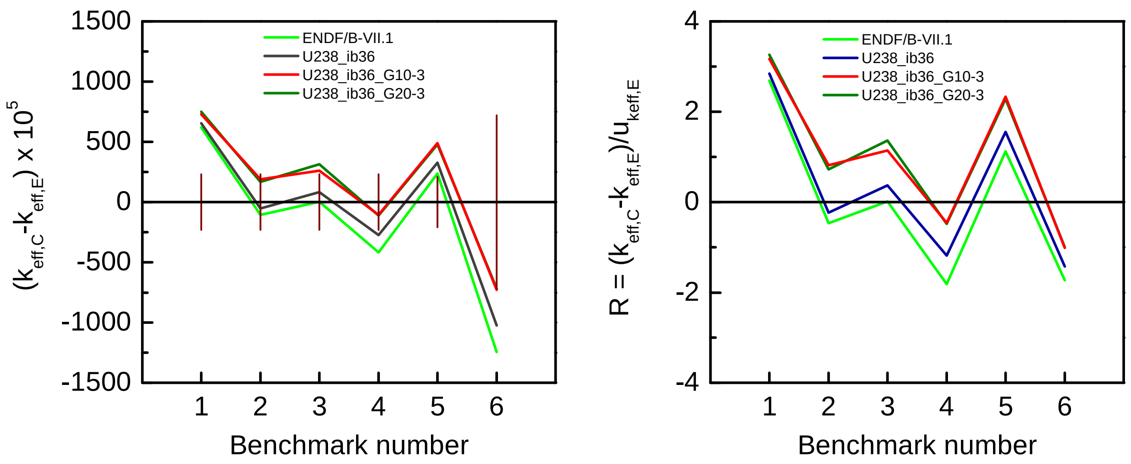

Figure 6 Difference between calculated and experimental reactivity (left) and the corresponding residuals for the benchmarks in Table 5. The experimental uncertainty is given in the left figure by the error bars.

Table 6. Average difference between calculated and experimental reactivity $<k_{eff,C} - k_{eff,E}>$ and χ^2-value defined in Eq. 3 derived from the 6 benchmarks listed in Table 5.

	$<k_{eff,C} - k_{eff,E}> \times 10^5$	χ^2
ENDF/B-VII.1	-152	15.0
U238_ib36	-48	14.1
U238_ib36_G10-3	140	18.7
U238_ib36_G20-3	147	19.5

A study of other benchmarks in Ref. [46] did not reveal notable differences, except for the benchmarks: IEU-MET-FAST-007 (Big Ten), IEU-MET-FAST-004 (VNII-CFT-4) and IEU-MET-FAST-010 (ZPR-6/9(U9)). For these benchmarks the calculated k_{eff} using the G20-3 based file was larger compared to the one obtained with the U238_ib36 file. The direct link to changes in the evaluation for ^{238}U has still to be investigated. It is worth noting that strong compensating effects of ^{235}U and ^{238}U evaluated data have been observed [47], therefore a full benchmark analysis requires also an updated evaluation of ^{235}U.

3.2.3 Validation by KAERI

A comprehensive study of the test files was carried out at KAERI [48]. A set of 94 criticality benchmark experiments containing ^{238}U was selected from the ICSBEP handbook [44]. The benchmarks are part of the expanded criticality validation suite for MCNP [49]. The experiments can be classified according to the composition of the fuel. Based on the main fuel component different categories can be identified: highly enriched uranium (HEU), intermediate enriched uranium (IEU), low enriched uranium (LEU), plutonium and ^{233}U. The MCNP5 code was used for calculations. These experiments, which are specified in Appendix C, were used to compare the performance of ENDF/B-VI.1, ENDF/B-VII.0, JEFF-3.2 and the test files presented in Table 4. For the test files JEFF-3.2 was taken as a base file.

The results of this exercise are summarised in Figure 7, Figure 8 and Table 7. They confirm that the $k_{eff,C}$ resulting from calculations based on the resonance parameter file of Derrien et al. [12] are more consistent with the experimental data compared to the $k_{eff,C}$ derived from ENDF/B-VI. The file of Derrien et al. [12] results in an overall increase of reactivity due to the reduction in thermal capture cross section and capture kernel. They also do not provide clear evidence that an increase in upper boundary of the RRR has a strong impact on the reactivity calculations.

For some experiments there is a substantial difference between results based on calculations with ENDF/B-VII.1 and JEFF-3.2 based files. Large differences are observed for the HEU-MET-INTER-006 (case 1 to 4) and MIX-MET-FAST-008-case-7 experiments. The HEU-MET-INTER-006 experiments contain a large amount of Cu. Since the difference increases with decreasing amount of graphite, the bias is most probably related to the cross sections for Cu. The resonance parameter files for Cu in ENDF/B-VII.2 and JEFF-3.2 are indeed different. The parameters of JEFF-3.2 are based on those obtained by Sobes [50]. Problems related to these parameters have already been reported in Ref. [51]. The difference observed for the MIX-MET-FAST-008-case-7 experiment has still to be clarified.

Differences between the different JEFF-3.2 based files are rather small. The results in Table 7 indicate that the overall best performance is obtained with the G20-4 file. It should be noted that in the calculations of the average difference and the χ^2 value the results of the HEU-MET-INTER-006 (case 1 to 4) experiments were not considered.

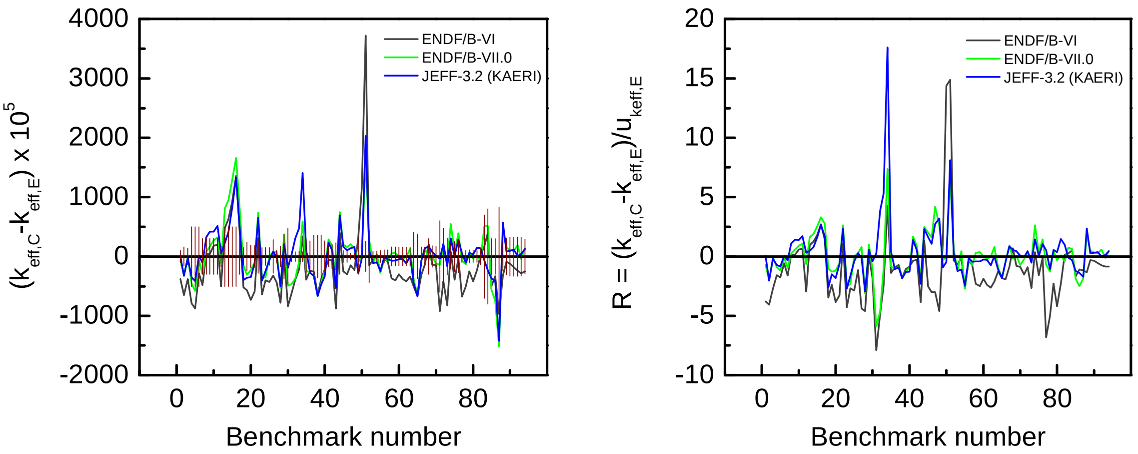

Figure 7 Difference between calculated and experimental reactivity (left) and the corresponding residuals for the benchmarks in Appendix C. The calculated reactivity is based on ENDF/B-VI, ENDF/B-VII.0 and JEFF-3.2. The experimental uncertainty is given in the left figure by the error bars.

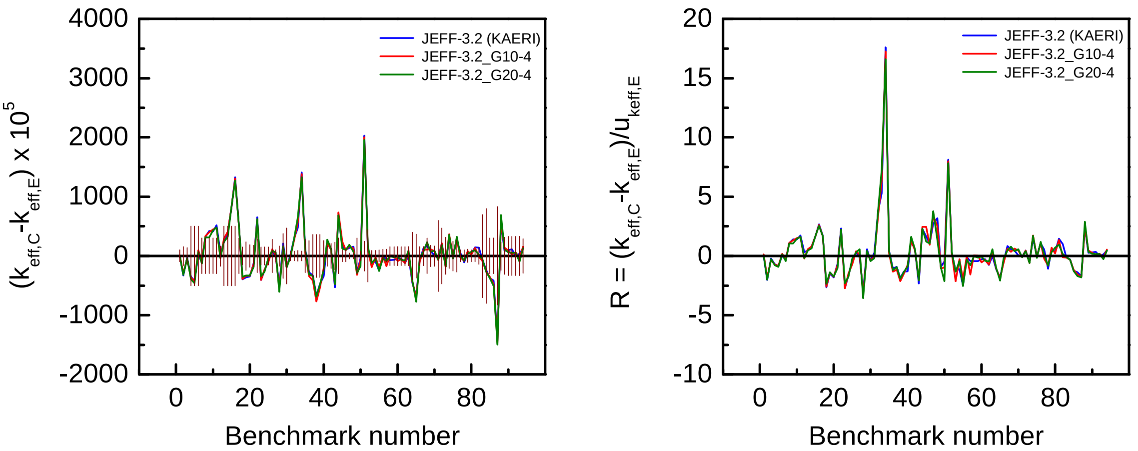

Figure 8 Difference between calculated and experimental reactivity (left) and the corresponding residuals for the benchmarks in Appendix C. The calculated reactivity is based on the JEFF-3.2 based file with different treatment of the URR. The experimental uncertainty is given in the left figure by the error bars.

Table 7. Average difference between calculated and experimental reactivity and χ^2 value defined in Eq. 3 derived from 90 benchmarks listed in Appendix C. The results for the heu-met-inter-006 experiments have not been considered in the calculations.

	$<k_{eff,C} - k_{eff,E}> \times 10^5$	χ^2
ENDF/B-VI	-180	220
ENDF/B-VII.0	33	271
JEFF-3.2 (KAERI)	10	213
JEFF-3.2_G10-1	18	248
JEFF-3.2_G20-1	23	257
JEFF-3.2_G10-2	8	229
JEFF-3.2_G20-2	12	221
JEFF-3.2_G10-3	11	230
JEFF-3.2_G20-3	4	219
JEFF-3.2_G10-4	4	217
JEFF-3.2_G20-4	2	210

4. Summary and recommendations

The improved performance of the parameter file for the resolved resonance region (RRR) proposed by Derrien et al. [12], which is adopted in the main data libraries, has been confirmed. These parameters are not fully consistent with the experimental transmission data of Olsen et al. [4-8]. Consistency with these data can be obtained by adjusting parameters of some bound states. Such an adjustment should be validated by additional transmission measurements and by an analysis of integral benchmark experiments with a high sensitivity to the thermal energy region, i.e. the experiments in Appendix A.

The cross section data for the unresolved resonance region (URR) in the main libraries are based on the work of Fröhner [23,24]. They slightly deviate from the average total cross section derived by Harvey et al. [13], which are based on transmission measurements at a 200 m station. Therefore, a new analysis including the data of Harvey et al. [13] should be carried out. Ideally an evaluated total cross section is derived from a least squares adjustment to the available experimental data, including the data of Ref. [13], and average resonance parameters, i.e. strength functions and scattering radii, are derived from an analysis of the resulting total cross section.

The results presented in this report show that an increase in upper boundary of the RRR from 10 keV and 20 keV is primarily needed when a high resolution group structure is required. In addition they suggest that a better performance is obtained when the infinitely diluted capture cross section is adopted from an analysis of the experimental data (Carlson et al. [35]) and the one for the inelastic scattering reaction is based on the one recommended by Capote et al. [38].

Despite the importance of the $^{238}U(n,\gamma)$ reaction for nuclear energy applications, there are no experimental cross section data available for this reaction that are consistent with recommended cross sections in both the RRR and URR.

The new experimental data should be included in a new evaluation for both the RRR and URR. The recommended fission widths should be consistent with the fission areas reported by Difilippo et al. [11]. In addition, full covariance data should be provided. To preserve the full uncertainties due to experimental effects, such as the normalization of capture data, the Monte Carlo approach proposed by De Saint Jean et al. [52] is recommended. Using methods based on conventional uncertainty propagation, the final uncertainty due to systematic effects can disappear, depending on the experimental conditions [42, 53].

The resulting file should be validated by the experiments mentioned in Ref. [43] and those presented in Appendix A, B and C, with a special emphasis on the IEU-MET-FAST-007, IEU-MET-FAST-004, IEU-MET-FAST-010 and MET-FAST-008-case-7 experiments and those in Appendix B with a high sensitivity to the cross sections in the region between 10 keV and 20 keV.

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Appendix A

Integral benchmark experiments with a high sensitivity to the cross section of ^{238}U in the thermal energy region

ICSBEP Id	Short name	Common name	MCNP input
LEU-MET-THERM-001			Y
LEU-MET-THERM-006-09	lmt006-09	Bugey 5	
LEU-MET-THERM-006-12	lmt006-12	Bugey 16	
LEU-MET-THERM-006-14	lmt006-14	Bugey 20	
LEU-MET-THERM-006-15	lmt006-15	Bugey 19	
LEU-MET-THERM-006-17	lmt006-17	Bugey 24	
LEU-MET-THERM-006-18	lmt006-18	Bugey 23	
LEU-MET-THERM-006-26	lmt006-26	Bugey 32	
LEU-MET-THERM-006-28	lmt006-28	Bugey 30	
LEU-MET-THERM-006-29	lmt006-29	Bugey 42	
LEU-MET-THERM-006-30	lmt006-30	Bugey 43	

Appendix B

Integral benchmark experiments with a high sensitivity to the cross section of ^{238}U in the energy region between 10 keV and 20 keV

ICSBEP Id	Common name	Reaction	Sensitivity* [(Δk/k)/(Δσ/σ] x 10^5
MIX-MISC-FAST-001-009	BFS-31-4	(n,tot)	-56
MIX-MISC-FAST-001-009	BFS-31-4	(n,γ)	-39
IEU-COMP-INTER-005-001	ZPR-6/6A	(n,γ)	-36
IEU-COMP-INTER-005-001	ZPR-6/6A	(n,tot)	-31
MIX-COMP-FAST-001-001	ZPR-6/7	(n,γ)	-31
MIX-COMP-FAST-006-001	ZPPR-2	(n,γ)	-29
MIX-COMP-FAST-005-001	ZPR-9 Ass 31	(n,γ)	-29
MIX-MISC-FAST-002-001	BFS-49/1A	(n,γ)	-
MIX-COMP-FAST-001-001	ZPR-6/7	(n,tot)	-27
MIX-COMP-FAST-006-001	ZPPR-2	(n,tot)	-26
MIX-COMP-FAST-005-001	ZPR-9 Ass 31	(n,tot)	-26
MIX-MISC-FAST-002-001	BFS-49/1A	(n,tot)	-
IEU-MET-FAST-017-001	BFS-35-1	(n,γ)	-20
MIX-MISC-FAST-001-011	BFS-42	(n,γ)	-20
IEU-MET-FAST-022-006	9-S	(n,γ)	-
IEU-COMP-FAST-004-001	ZPR-3/12 Load 10	(n,γ)	-20
IEU-MET-FAST-017-001	BFS-35-1	(n,tot)	-20
MIX-MISC-FAST-001-011	BFS-42	(n,tot)	-20
IEU-MET-FAST-022-006	9-S	(n,tot)	-
MIX-MISC-FAST-003-001	BFS-97/1	(n,γ)	-17
MIX-MISC-FAST-003-001	BFS-97/1	(n,tot)	-12
IEU-MET-FAST-022-005	8-S	(n,γ)	-
MIX-MET-INTER-004-001	ZPR-3/53	(n,γ)	-15
IEU-MET-FAST-010-001	ZPR-6/9 Load11	(n,γ)	-15
IEU-COMP-FAST-004-001	ZPR-3/12 Load 10	(n,tot)	-15
IEU-MET-FAST-022-005	8-S	(n,tot)	-
IEU-MET-FAST-022-007	10-S	(n,γ)	-
IEU-MET-FAST-012-001	ZPR-3/41	(n,γ)	-14
IEU-MET-FAST-010-001	ZPR-6/9 Load11	(n,tot)	-13
IEU-MET-FAST-022-001	3X-S	(n,γ)	-
IEU-MET-INTER-001-002	5-S	(n,γ)	-
IEU-MET-FAST-022-001	3X-S	(n,tot)	-
IEU-MET-FAST-022-007	10-S	(n,tot)	-
IEU-MET-INTER-001-003	6A-S	(n,γ)	-
IEU-MET-INTER-001-004	7-S	(n,γ)	-

* Sensitivities calculated by NDaST (http://www.oecd-nea.org/ndast/)

Appendix C

Integral benchmark experiments which have been analysis at KAERI [48]. The first column is used as identification number in Figure 7 AND Figure 8.

Experiment number	ICSBEP identification	$k_{eff,E}$	$u_{keff,E}$
1	heu-met-fast-001	1.0000	0.0010
2	heu-met-fast-008	0.9989	0.0016
3	heu-met-fast-018-case-2	1.0000	0.0014
4	heu-met-fast-003-case-1	1.0000	0.0050
5	heu-met-fast-003-case-2	1.0000	0.0050
6	heu-met-fast-003-case-3	1.0000	0.0050
7	heu-met-fast-003-case-4	1.0000	0.0030
8	heu-met-fast-003-case-5	1.0000	0.0030
9	heu-met-fast-003-case-6	1.0000	0.0030
10	heu-met-fast-003-case-7	1.0000	0.0030
11	heu-met-fast-028	1.0000	0.0030
12	heu-met-fast-014	0.9989	0.0017
13	heu-met-fast-003-case-8	1.0000	0.0050
14	heu-met-fast-003-case-9	1.0000	0.0050
15	heu-met-fast-003-case-10	1.0000	0.0050
16	heu-met-fast-003-case-11	1.0000	0.0050
17	heu-met-fast-003-case-12	1.0000	0.0030
18	heu-met-fast-013	0.9990	0.0015
19	heu-met-fast-021-case-2	1.0000	0.0024
20	heu-met-fast-022-case-2	1.0000	0.0019
21	heu-met-fast-012	0.9992	0.0018
22	heu-met-fast-019-case-2	1.0000	0.0028
23	heu-met-fast-009-case-2	0.9992	0.0015
24	heu-met-fast-009-case-1	0.9992	0.0015
25	heu-met-fast-011	0.9989	0.0015
26	heu-met-fast-020-case-2	1.0000	0.0028
27	heu-met-fast-004-case-1	1.0020	0.0010
28	heu-met-fast-015	0.9996	0.0017
29	heu-met-fast-026-case-c-11	1.0000	0.0038
30	heu-comp-inter-003-case-6	1.0000	0.0047
31	heu-met-inter-006-case-1	0.9977	0.0008
32	heu-met-inter-006-case-2	0.9997	0.0008
33	heu-met-inter-006-case-3	1.0015	0.0009
34	heu-met-inter-006-case-4	1.0016	0.0008
35	u233-comp-therm-001-case-6	1.0015	0.0028
36	heu-sol-therm-013-case-1	1.0012	0.0026
37	heu-sol-therm-013-case-2	1.0007	0.0036
38	heu-sol-therm-013-case-3	1.0009	0.0036
39	heu-sol-therm-013-case-4	1.0003	0.0036
40	heu-sol-therm-032	1.0015	0.0026
41	ieu-met-fast-003-case-2	1.0000	0.0017
42	ieu-met-fast-005-case-2	1.0000	0.0021
43	ieu-met-fast-006-case-2	1.0000	0.0023
44	ieu-met-fast-004-case-2	1.0000	0.0030
45	ieu-met-fast-001-case-1	0.9989	0.0010
46	ieu-met-fast-001-case-2	0.9997	0.0010
47	ieu-met-fast-001-case-3	0.9993	0.0005
48	ieu-met-fast-001-case-4	1.0002	0.0005
49	ieu-met-fast-002	1.0000	0.0030
50	ieu-met-fast-007-case-4	1.0049	0.0008

Experiment number	ICSBEP identification	$k_{eff,E}$	$u_{keff,E}$
51	mix-met-fast-008-case-7	1.0030	0.0025
52	ieu-comp-therm-002-case-3	1.0017	0.0044
53	leu-sol-therm-007-case-14	0.9961	0.0009
54	leu-sol-therm-007-case-30	0.9973	0.0009
55	leu-sol-therm-007-case-32	0.9985	0.0010
56	leu-sol-therm-007-case-36	0.9988	0.0011
57	leu-sol-therm-007-case-49	0.9983	0.0011
58	leu-comp-therm-008-case-1	1.0007	0.0016
59	leu-comp-therm-008-case-2	1.0007	0.0016
60	leu-comp-therm-008-case-5	1.0007	0.0016
61	leu-comp-therm-008-case-7	1.0007	0.0016
62	leu-comp-therm-008-case-8	1.0007	0.0016
63	leu-comp-therm-008-case-11	1.0007	0.0016
64	leu-sol-therm-002-case-1	1.0038	0.0040
65	leu-sol-therm-002-case-2	1.0024	0.0037
66	mix-met-fast-001	1.0000	0.0016
67	mix-met-fast-003	0.9993	0.0016
68	pu-met-fast-006	1.0000	0.0030
69	pu-met-fast-010	1.0000	0.0018
70	pu-met-fast-020	0.9993	0.0017
71	mix-comp-therm-002-case-pnl30	1.0024	0.0060
72	mix-comp-therm-002-case-pnl31	1.0009	0.0047
73	mix-comp-therm-002-case-pnl32	1.0042	0.0031
74	mix-comp-therm-002-case-pnl33	1.0024	0.0021
75	mix-comp-therm-002-case-pnl34	1.0038	0.0025
76	mix-comp-therm-002-case-pnl35	1.0029	0.0027
77	u233-met-fast-001	1.0000	0.0010
78	u233-met-fast-002-case-1	1.0000	0.0010
79	u233-met-fast-002-case-2	1.0000	0.0011
80	u233-met-fast-003-case-1	1.0000	0.0010
81	u233-met-fast-003-case-2	1.0000	0.0010
82	u233-met-fast-006	1.0000	0.0014
83	u233-met-fast-004-case-1	1.0000	0.0070
84	u233-met-fast-004-case-2	1.0000	0.0080
85	u233-met-fast-005-case-1	1.0000	0.0030
86	u233-met-fast-005-case-2	1.0000	0.0030
87	u233-sol-inter-001-case-1	1.0000	0.0083
88	u233-comp-therm-001-case-3	1.0000	0.0024
89	u233-sol-therm-001-case-1	1.0000	0.0031
90	u233-sol-therm-001-case-2	1.0000	0.0033
91	u233-sol-therm-001-case-3	1.0000	0.0033
92	u233-sol-therm-001-case-4	1.0000	0.0033
93	u233-sol-therm-001-case-5	1.0000	0.0033
94	u233-sol-therm-008	1.0000	0.0029

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